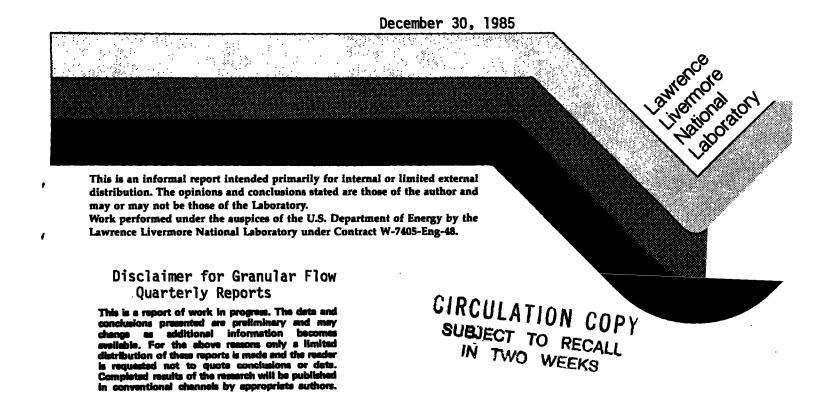
LAWRENCE LIVERMORE NATIONAL LABORATORY GRANULAR FLOW PROJECT - QUARTERLY REPORT

October - December 1985

Edited by O. R. Walton

For
U.S. Department of Energy
Office of Fossil Energy
Pittsburgh Energy Technology Center
Pittsburgh, Pennsylvania



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Granular Flow Project - Quarterly Report October - December 1985 O.R. Walton, Editor

LLNL's Granular Flow Project is developing and utilizing new discrete particle computer models to determine the rheologic characteristics of idealized granular solids under various flow conditions. During FY85 two-dimensional granular material models of assemblies of inelastic. frictional, circular disks were developed and utilized in various parameter studies. During the current reporting period we completed an initial parameter study of steady shearing flows of idealized granular materials consisting of assemblies of equal-sized, inelastic spheres. The results of this study have been submitted for publication in Acta Mechanica. Our three-dimensional computer model has also been extended to include frictional interactions between spherical particles. A calculational series is underway examining the effects of interparticulate friction and rotations on the stresses in steady shearing flows. New post processing routines have also been written that provide the cabability of making multi-color three-dimensional perspective-projection motion pictures of the granular flow calculations. We report below the highlights of the work performed during this first quarter of FY86.

3-D Shearing Flow Calculations -- Inelastic Spheres

The 3DSHEAR model, described previously [1], was utilized in a parameter study examining the effects of inelasticity on the stresses in uniformly shearing assemblies of equal-sized, inelastic spheres. The molecular-dynamics-like calculations consisted of a primary calculational cell containing 125 inelastic spheres with periodic boundaries on all sides. Particles (or periodic images) located one cell height above or below their images in the primary cell are moved to the right or left respectively, forcing a uniform shearing motion throughout the entire assembly. This simulates the kind of motion that would be experienced by a small cubical cell of granular material within a larger region undergoing steady shearing flow, such as can occur in annular shear cells, in incline chute flows and in other configurations. This initial parameter study examined the effects of coefficient-of-restitution, solids-packing-fraction and shear-rate on the mean stresses and deviatoric velocities in a granular assembly. The effects of boundary interactions and energy coupling from real boundaries will be the subject of future investigations as will be an investigation of the effects of interparticulate friction and particle rotations. Both constant coefficient-of-restitution and variable coefficient-of-restitution interactions were modeled using a partially-latching spring model analogous to the normal-force model used in previously reported two-dimensional studies [2]. The constant coefficient of restitution calculations resulted in behavior quite similar to the predictions of a linearized perturbation to Chapman-Enskog theory for slightly inelastic spheres by Lun et al. [3]. We found that the calculated stresses increased almost in direct proportion to the square of the shear rate for solids packing fractions, ν , in the range $0.1 < \nu < 0.5$. At higher solids concentrations, where enduring contacts occur, the computer-simulated flows showed a less rapid variation with shear rate and

at very low solids concentrations the calculated stresses increased somewhat faster than the square of the strain rate. As the solids packing decreased and as the inelasticity of the interactions became more pronounced the calculated deviatoric velocity distributions became quite anisotropic with much larger components in the direction parallel to the shear than in the directions perpendicular to the shear. Consequently the calculated normal stress component parallel to the shearing direction, $p_{\chi\chi}$, also became significantly larger than the normal stress components perpendicular to the shear, $p_{\chi\chi}$ and $p_{\chi\chi}$. Such behavior was also seen in our previous two-dimensional calculations but has generally not been included in current microstructural theories describing granular solids.

The similarity between our calculated stresses and those of the Lun et al. theory can be seen in Figure 1. This figure shows the calculated shear stress, $\mathbf{p}_{_{\boldsymbol{X}\boldsymbol{V}}}\text{, for systems composed of spheres with constant coefficients of$ restitution, e, of 0.95, 0.80, and 0.60 (symbols and solid line), and the predictions of the Lun et al. theory (dashed lines). The values in this figure have been non-dimensionalized by dividing by $\rho_n \sigma^2 \hat{\epsilon}$, where $ho_{
m D}$ is the solid material density, σ is the sphere diameter and $\dot{\epsilon}$ = du_x/dy is the shear rate. Also shown is the calculated shear stress obtained with a variable coefficient of restitution model. In the solids fraction range 0.1 < v < 0.5 the calculated values of the present work are generally within ~10% of the Lun et al. theory for e = 0.95, within ~20% for e = 0.80 and within about 40% for e = 0.60. At extremes in solids concentrations more substantial differences occur. Such differences are not unexpected since the theory assumes only binary collisions, an assumption not valid at high solids concentrations, and it further assumes an isotropic deviatoric velocity distribution, a condition not found at low solids concentrations in the calculations.

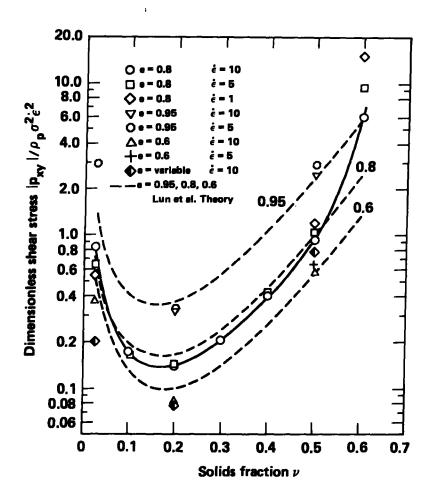


Figure 1. Calculated variation of dimensionless shear stress with solids fraction for system of 125 inelastic spheres in uniform shearing flow (symbols); _____ spline fit to e=0.8, $\dot{\epsilon}=10$ case; ____ Lun et al. theory [3].

The calculated variation of the ratio of shear-stress to normal stress, $|p_{xy}/p_{yy}|$, with solids fraction is shown in Figure 2 for spheres interacting with constant coefficients of restitution of e = 0.95, 0.80, and 0.60 and also for a variable-e interaction. The calculated value of $|p_{xy}/p_{yy}| \simeq 0.2$ for e = 0.95 is very close to the Lun et al. theory also shown on Figure 2. At lower coefficients of restitution the

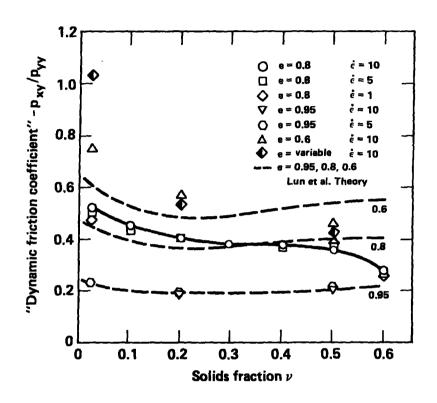


Figure 2. Calculated variation of dynamic friction coefficient $|p_{XY}/p_{YY}|$ with solids fraction for a system of 125 inelastic spheres in uniform shearing flow (symbols); spline fit to e = 0.8, ε = 10 calculated points Lun et al. theory [3].

calculated and theoretical values for this "dynamic friction coefficient" show some deviation. Both the theretical values due to Lun et al. and our calculations of $|p_{xy}/p_{yy}|$ are significantly smaller than the measured values for this stress ratio (in the range between 0.5 and 0.7) obtained in annular shear cell tests with glass beads and polystyrene beads ([4],[5]). Preliminary calculations, currently in progress, examining the

effects of friction and particle rotations, are producing shear stress to normal stress ratios in the range of those experimentally measured values. During the next reporting period we plan to continue the investigation of the effects of friction and particle rotations on the calculated stresses and will report the results when the work is further along. The results of the initial parameter study of inelastic spheres are more completely described in a paper submitted for publication [6] in a special issue of Acta Mechanica devoted to granular materials, scheduled for publication late in the spring of 1986.

Friction Force Added to 3DSHEAR Model

A tangential friction force model analagous to the incrementally-slipping friction model used in previous two-dimensional calculations [2] has been added to the 3DSHEAR calculational code. The model accounts for tangential sliding friction during impacts in a manner very similar to that of Mindlin and Deresiewicz [7]. A series of planar two-body impact calculations with head-on and glancing collisions including non-rotating and initially rotating spheres has verified that for planar impacts this three-dimensional model produces post collisional trajectories and rotations that are essentially identical to those obtained with the previous two-dimensional model. A shearing flow parameter study is in progress examining the effects of tangential sliding friction between inelastic spheres on the stresses and deviatoric velocity distributions obtained. Preliminary results from that study (consistent with earlier two-dimensional results) indicate that at high solids concentrations interparticulate friction increases shear stresses, but does not greatly affect the normal stress. At very low solids packings the major effect of the friction is to provide an additional energy loss mechanism during

two-body collisions so that all stress components are reduced. We anticipate that the stresses obtained in this calculational study will be very similar to those measured in laboratory tests of glass and polystyrene beads [4,5].

For non-planar binary collisions it is possible for relative sphere rotations about the line joining their centers to affect the frictional forces acting between the particles through both a "spin-coupling" term and by a modification to the tangential sliding friction force. Neither of these "second order" friction interaction terms are included in the present friction model. We do not expect that they will greatly affect calculated stresses in shearing assemblies, but we do plan to investigate the feasibility of including such effects in our particle interaction models so that sensitivity studies can be performed.

3-D Graphics and Post Processing Improved

The post processing graphics routine for the 3DSHEAR model has been modified to plot the particles in the primary calculational cell and also the periodic image particles in the cell located immediately below the primary cell. The plotting routine was also modified to plot only the portion of each sphere that is inside the cell (i.e. fractional spheres are plotted if they intersect an edge of the calculational cell). Both orthographic projection and perspective projections can be plotted in black and white or in color. Figure 3 is an example frame from a perspective projection movie of a shearing flow calculation showing 125 particles in the primary cell and their images in the cell immediately below the primary cell. In addition to position plots the post-processing graphics routine also can generate time history plots of any of nearly 50 quantities averaged

over the entire cell or over each of several vertical zones spanning the cell. The generation of color, perspective-projection movies of the particle positions during a steady state shearing flow calculation takes significant amounts of computer time; thus it is not a routine post processing procedure. These movies are used, along with the zonal averages of the velocity field, to verify that uniform shearing is occuring in the calculations at high solids packing fractions. In previous two-dimensional calculations these position plots were extremely useful in determining the maximum solids packing that still resulted in uniform shearing instead of a single shearing layer. We expect them to be equally valuable in three dimensions.

••time = 3.8000e-01

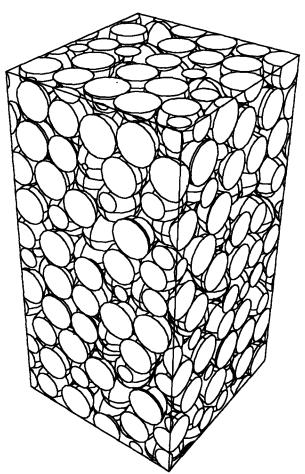


Figure 3.

Snapshot of 125 particles in steady shearing flow calculation.

Visitors:

T. Anthony Royal, Vice President, Jenike & Johanson (an engineering consulting firm specializing in bulk solids flow problems)

November 14,1985; to tour Laser Fusion and Oil Shale facilities and discuss granular solids research.

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